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## Distribution of ferromagnetic moments in crystals under external twisting

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## ABSTRACT

In an easy-axis ferromagnet, the effect of superposition of severe plastic deformation by twisting (SPDT) perpendicular to the “easy axis” on the ferromagnetic order parameter (OP) distribution is studied. The consideration is carried out within the frameworks of phenomenological theory of Landau. It is shown that SPDT effects the results in occurrence of the normal component of the magnetic OP and periodical change of OP modulus. The law of distribution of the magnetic moment is determined by proximity of the temperature of the crystal and any phase transition.

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## 1. Introduction

Interaction of structural and magnetic order parameters (OPs) has been investigated long enough. The work [1] should be mentioned in particular, where two interacting OPs were considered and phase diagrams were constructed in the space of coefficients of non-equilibrium thermodynamic potential (NETP). This approach was developed further in a number of studies [2–4]. In particular, in [2], within the frameworks of the Landau theory, diagrams of structural and magnetic phase transitions (PT) were theoretically analyzed in the ferromagnetic Ni–Mn–Ga alloy with the shape memory effect allowing for modulation OP. It was demonstrated that in this case, both martensitic transformations and pre- and after-martensitic transitions can occur, being related to appearance of modulated structure. The deformation and modulation OPs interact with the magnetic OP, so they substantially affect the magnetic PT.

In [3] theoretical analysis of the effect of the external magnetic field on PT in Heisler’s alloys of Ni–Mn–X (X=In, Sm, Sb) was conducted. It was shown that external magnetic field substantially shifts the temperature of a bound magneto-structural PT. The previous studies mentioned above, however, did not deal with the effect of applied external mechanical impact on the OP distribution and the change in PT temperatures. In [4], the effect of severe

plastic deformation by twisting on the properties and the structure of the Ni<sub>24</sub>Mn<sub>21</sub>Ga<sub>25</sub> and Ni<sub>24</sub>Mn<sub>20</sub>FeGa<sub>25</sub> was considered. It was demonstrated that atomic disordering and structuring of these alloys under external effects result in suppression of reversible magnetically controlled shape memory effects. The effect of bend-induced anisotropy on spin wave spectrum in a magnetic nanowire twisted as a screw line was considered in [5]. There, a nanowire with constant and cycling step was used. It was shown in [6] that the Pt<sub>3</sub>Fe alloy transformed from antiferromagnetic state to the ferromagnetic one as a result of severe plastic deformation by twisting under high pressure. Investigation of distribution of the modulus of structural OP and its forced alteration under periodical changes of the modulus of magnetic OP in the phase with the spiral structure [7] was carried out in [8]. The inverse problem of describing the effect of severe plastic deformation by twisting (SPDT) along the axis of the rod on the distribution of ferromagnetic order parameter in the crystal is of equal interest and it is presented in this work.

## 2. Theory

Let us suggest that the torsion moment of SPDT is applied to a model ferromagnetic, square with the “easy axis” OZ. The appearing deformation related to the rotation of the structural order parameter (OP) in XOZ plane will be further called twist deformation. The ferromagnetic order parameter formed by a superposition of elementary moments of ions of an elementary cell is

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located in the plane of rotation of the structural OP. The last one is a linear combination of deviations of ions in an elementary cell. The structural OP can be forced if the crystal temperature is above the temperature of the structural PT. To describe this system theoretically, it is usable to expand formalism applied by Dzyaloshinski to long-range spiral magnetic structures [9] to the case of SPDT. When using this method, appeared inhomogeneity of distribution of the corresponding OP is considered in a non-equilibrium thermodynamic potential (NETP) as the first spatial derivative. Thus, the selected configuration can be represented by the following NETP:

$$\begin{aligned} \Phi = & \frac{\alpha_1}{2}q^2 + \frac{\alpha_2}{4}q^4 + \frac{\alpha_3}{6}q^6 + \frac{\beta_1}{2}F_z^2 + \frac{\beta_2}{4}F_z^4 + \frac{\beta_3}{6}F_z^6 \\ & + \frac{\beta_4}{2}F_x^2 + \frac{\beta_5}{4}F_x^4 + \gamma_1q^2(F_x^2 + F_z^2) + \gamma_4F_x^2F_z^2 \\ & - \gamma_2M^r \left( q_z \frac{\partial q_x}{\partial y} - q_x \frac{\partial q_z}{\partial y} \right) + \gamma_3M^s \left( \left( \frac{\partial q_x}{\partial y} \right)^2 + \left( \frac{\partial q_z}{\partial y} \right)^2 \right) \end{aligned} \quad (1)$$

here  $\alpha_i, \beta_i, \gamma_i$  are phenomenological constants,  $\vec{q}$  and  $\vec{F}$  are structural and ferromagnetic order parameters. OZ axis is directed along the “easy axis”, rotation occurs in XZ plane, OY is the rotation axis. It was suggested in (1) that  $\alpha_1, \beta_1, \beta_4$  are temperature dependent and alternate the sign at the critical points,  $\alpha_3 > 0, \beta_3 > 0, \beta_5 > 0, \gamma_1 < 0, \gamma_4 < 0, \beta_4 > 0$ . The signs of the rest of the coefficients will be changed at formulation of the computing experiment. Potential (1) requires accounting for the elastic and magnetoelastic interactions. Being different from zero, tensor components that describe these interactions can be eliminated when their equilibrium values depending on the value of the structural and the magnetic order are estimated with the aid of the equations of state. After the substitution of the found relations in the potential, a new potential formally coincides with NETP without considering elastic and magnetoelastic interactions. At the same time, new re-normalized constants will be pressure and temperature dependent. Further we will suppose that the procedure of elimination has been accomplished.

The terms with spatial derivatives describe the twist deformation (disproportionate long-periodic spiral structure) and contain a multiplier proportional to the moment  $M$ , i.e. spatial spiral structure is absent at  $M = 0$ . If  $\alpha_i$  ( $i = 1, 2, 3$ ),  $\beta_i$  ( $i = 1-5$ ),  $\gamma_1, \gamma_4$  are equal to zero, the corresponding Euler's equation with approximation of OP modulus constancy  $\vec{q}$  has the solution in the form of a structural periodic spiral described by the relations:

$$\begin{cases} q_x = |q| \cos(ky) \\ q_z = |q| \sin(ky) \end{cases} \quad (2)$$

where  $k$  is the propagation vector directed along OY axis. After combining (2) and (1) and differentiating with respect to  $k$ , the value for the propagation vector modulus can be found:

$$k = \frac{\gamma_2 M^{r-s}}{2\gamma_3} \quad (3)$$

It follows from (3) that  $r > s$ , because  $k$  must increase with the increase in  $M$ . To verify this statement and to estimate the magnitude of the difference  $r-s$ , a special experiment was carried out. Iron wire of 3 mm in diameter and 100 mm in length was exposed to SPDT with varied moments. At the same time, the turning angle of a fixed point on the surface of the wire was measured. The results are listed in the Table 1. The obtained experimental results are well approximated by the Eq. (3) at  $r-s = 4$  and  $\gamma_2/(2 \times \gamma_3) \sim 1, 14 \times 10^{-7}$ . In the present work, the parameters are set as  $r = 6, s = 2$ .

If we suggest that modules of irreducible vectors are not constant, the system of Euler's equation is obtained

$$\begin{cases} 2\gamma_3 M^s \frac{\partial^2 q_x}{\partial y^2} + 2\gamma_2 M^r \frac{\partial q_x}{\partial y} - q_x [\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\gamma_1 (F_x^2 + F_z^2)] = 0 \\ 2\gamma_3 M^s \frac{\partial^2 q_z}{\partial y^2} - 2\gamma_2 M^r \frac{\partial q_z}{\partial y} - q_z [\alpha_1 + \alpha_2 q^2 + \alpha_3 q^4 + 2\gamma_1 (F_x^2 + F_z^2)] = 0 \\ \beta_1 + \beta_2 F_z^2 + \beta_3 F_z^4 + 2\gamma_1 q^2 + 2\gamma_5 F_x^2 = 0 \\ \beta_4 + \beta_5 F_x^2 + 2\gamma_1 q^2 + 2\gamma_5 F_z^2 = 0 \end{cases} \quad (4)$$

The similar system of equations subject to the single OP ( $\vec{q}$ ) has the solution in the form of long-range spatial structure. Such structure was studied in [10] with using of OP modulus constancy approximation. It permitted to solve the system of Euler's equation analytically. In addition, the Fourier analysis has been fulfilled, because solution was expansion into a series of limited number of multiple harmonic components. Such approach does not allow to obtain the spatial distribution of OP modulus and to show the spatial amplitude and frequency modulation of long-period spiral structure. These peculiarities can be noticed only with using numerical solution of Euler's equation system [7]. In this case with the help of Fourier analysis, the presence of the aliquant and rather large harmonic components may be detected. Therefore the system of differential-algebraic equations was solved numerically with help of MathLab 7 package with using of singular matrix of mass. The results of calculations are presented below.

### 3. Computation experiment

#### 3.1. Results and discussion

Let's suppose that the structural and magnetic phase transformation at different temperatures take place in the crystals. According to the phenomenological theory, quadratic coefficients of OP depend on the temperature difference in the crystal and the corresponding critical temperature. The type of PT becomes apparent at a temperature below the critical value and the sign of this coefficient changes from positive to negative. The type of PT is determined by the sign of the coefficient ( $\alpha_2, \beta_2$ ) at the fourth power of the OP. If the coefficient is positive, then the corresponding equation of state at the point of PT has only the zero solution and the PT is the transformation of the second order. If it is negative, then there is a nonzero solution, and we have a first-order phase transformation. In accordance with this, look at the various combinations of the two phase transformation and behavior of structural and magnetic order parameters as a function of temperature for different values of the NETP phenomenological parameters. Such an approach will allow the application of the obtained results to a wide range of crystals. It should be noted that the numerical calculations were performed in relative units. Therefore small values were considered as value of the order of unity. Value at which the graphs topology significantly changed, was considered as large. In this case, the ratio of these values is about 10.

Let us consider the behavior of the structural and magnetic OPs at some values of phenomenological parameters of NETP.

- (1)  $\alpha_1 < 0, \alpha_2 < 0, \alpha_3 > 0, \beta_1 > 0, \beta_2 > 0, \beta_3 > 0, \beta_4 > 0, \beta_5 > 0, \gamma_1 < 0, \gamma_2 > 0, \gamma_3 > 0, \gamma_4 < 0, M > 0$ . This set of inequalities for the coefficients means that the temperature of the crystal is below the line of the structural first-order phase transition but above the line of the magnetic second-order phase transition.

**Table 1**  
Experimental loading dependence of the turning angle.

Moment, $M$ (kNm)	0	50	70	85	90	95
Turning angle (deg.)	0	10	25	50	75	90

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